

## ABSTRACT

After first establishing that the MEAM interatomic potential [1] produced brittle fracture in silicon [2], we simulated implantation in silicon using molecular dynamics (MD). Ion implantation produced nanoclusters of disordered atoms, which was confirmed with TEM. The presence of these clusters allowed silicon to deform plastically as a crack approached, blunting the crack tip and arresting crack growth. The MD calculations show that the fracture toughness increases by a factor of 3. We have conducted experiments with silicon implanted with Ne and Xe ions. Experimentally measured increases in fracture toughness support the MD predictions.

## MOTIVATION

Currently, the strength of structural members in MEMS devices is limited by failure caused by fracture at surface flaws. In order to double the strength of the member, the critical stress intensity factor must be increased by a factor of two or the minimum flaw size must be decreased by a factor of four. The latter approach would require the development of completely new technology.



$$K_{IC} = 1.4\sigma_c\sqrt{a}$$

## CHARACTERIZATION

RBS-channeling and TEM results show that the density of nanocluster defects increases with dose. Implanter region eventually becomes fully amorphous.

Increasing the dose increases the amount of damage, but decreases fracture toughness. Similar effects were also seen in the MD simulations. Spectrums shown are for implantation with 100, 200 and 300 keV Ne ions.